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Consistency and Cluster Size in the Effective Field Theories of Ferromagnetism

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It is a well known fact that the Bethe-Peierls-Weiss (BPW) method which treats a central spin and all of its nearest neighbors gives much better Curie temperatures than the molecular field theory or Oguchi method which treat smaller clusters (1). However, the effectiveness of the BPW method lies not only in the size of the cluster but also in its consistency condition. This will be demonstrated by treating a consistent three-cluster.

In the effective field theories some of the interactions of a central spin S_o are taken into account exactly in the Hamiltonian while the other interactions are replaced by some effective field. The BPW Hamiltonian for a cluster without an external magnetic field is

$$H = -2JS_o \sum_{i=1}^{n} S_i - h_1 \sum_{i=1}^{n} S_i^z ,$$

where J is the exchange constant, n is the number of nearest neighbors, and h_1 is an effective field acting on the neighbors of S_o. h_1 is determined by requiring that the average value of S^z be the same for S_o as for its neighbors. This consistency requirement is

$$\langle S_o^z \rangle = \frac{1}{n} \left\langle \sum_{i=1}^{n} S_i^z \right\rangle .$$

We now treat an open three-cluster in which we take into account exactly only the interactions between a central spin and two of its nearest neighbors which are not nearest neighbors to each other. The Hamiltonian for such a cluster is

$$H = -2JS_o(S_1 + S_2) - A_oS_o - A_1(S_1^z + S_2^z) ,$$

where A_o and A_1 are effective fields, A_o acting on the central spin and A_1 on two of its neighbors. Oguchi (2) generalized molecular field theory to this cluster by assuming

$$A_o = -2J(n-2)\frac{1}{3}\left\langle S_o^z + S_1^z + S_2^z\right\rangle$$

$$A_1 = -2J(n-1)\frac{1}{3}\left\langle S_o^z + S_1^z + S_2^z\right\rangle .$$

The Oguchi theory is not consistent, in that $\left\langle S_o^z\right\rangle$ is not equal to $\left\langle S_1^z\right\rangle$ or $\left\langle S_2^z\right\rangle$.

If, instead of making Oguchi's entire assumption, we only assume that the effective field is proportional to the number of interactions which it replaces, i.e.,

$$\frac{A_o}{n-2} = \frac{A_1}{n-1} ,$$

then we can also require consistency,

$$\left\langle S_o^z\right\rangle = \frac{1}{2}\left\langle S_1^z + S_2^z\right\rangle .$$

The calculation is similar to that for the BPW method and yields in the case of spin 1/2 the following equation for the Curie temperature:

$$j_c = \frac{8}{9}\,\frac{\exp(j_c) - 1}{(n-2)\exp(2j_c) + (\frac{2}{3} - n)} ,$$

where $j_c = J/kT_c$ and T_c is the Curie temperature. Table 1 gives j_c for the simple and body-centered cubic lattices.

Table 1

j_c for spin 1/2

	n = 6	n = 8
Oguchi (second approx.)	0.356	0.259
Consistent three-cluster	0.560	0.348
BPW	0.541	0.344

From the table it is seen that the consistency condition has caused the three-cluster to give results very close to those of the full BPW cluster. Thus it appears that consistency is a stronger point in favor of the BPW method than large cluster size.

References

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(2) T. OGUCHI, Progr. theor. Phys. (Kyoto) 13, 148 (1955).

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